Advanced Monte Carlo: reweighting and parallel tempering

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Contents

1 Before you start

Download the files from the tutorial webpage, unpack them, cd to the `parallel_tempering` directory and execute the following command:

```
./run_pt.sh
```

The script will execute a parallel tempering simulation with some pre-defined parameters. It will keep your computer busy for a couple of minutes and provide you with some time to study the rest of the worksheet and the included files. If it does not run out of the box, read further about how to compile `ising_pt` and then try again.

The enclosed sources and programs

Each program has its own subdirecotry. We provide pre-compiled binary executables, which should run out of the box on computers in the CIP pool. If they do not run, cd to the corresponding directory, remove the executable and execute `make`. If even

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this fails, edit the makefile and remove the `-O3` option from the compile command. As usual, all programs print usage information when invoked without arguments or with an inappropriate numer of arguments.

`ising` Is our old known ising simulation program.

`ising_pt` Is a modification of the ising program which performs the parallel tempering simulation at a given set of temperatures. Its output is the energy per site and magnetization per site for the whole series of temperatures. The average values are printed to screen and the time series are stored in two files `magnetization.dat` and `energy.dat`.

`histogram` Makes a histogram of values in a selected column of a file.

`reweight` Does the reweighting from a reference temperature to a range of target temperatures, based on the time series of energy and observable values (per lattice site). As an input, the time series of the energies and the corresponding time series of the observables is required.

`run_pt.sh` Is a shell script which executes the simulation program and feeds it with the desired arguments

Homework 1 (2 points)

In the following, just explain in words, what you would expect for the 2D Ising model, without running the simulations.

1. What should be the average absolute value of magnetization per site, $\langle |m| \rangle$, at the following temperatures: $T \ll T_{\mathrm{c}}$, $T \approx T_{\mathrm{c}}$ and $T \gg T_{\mathrm{c}}$?

2. What should be the average value of magnetization per site, $\langle m \rangle$ at the same temperatures? Consider, that because of symmetry, values of m and $-m$ are equally probable.

3. How would the probability distribution of m change when going tom $T \ll T_{\mathrm{c}}$ to $T \gg T_{\mathrm{c}}$?

4. How would the probability distribution of energy per site, e, change when going tom $T \ll T_{\mathrm{c}}$ to $T \gg T_{\mathrm{c}}$?
   Hint: To get a better clue about answers to several questions from this worksheet, it may be useful to tead the article by Janke [1] Note that it is not the same as previously..

2 Reweighting

In the reweighting procedure, we use simulation data obtained at a reference temperature T_0 to compute averages of observables at a different temperature T. The average of a

quantity which is a function of energy at a given temperature T, $\langle f(E) \rangle (T)$ is then obtained from the formula

$$\langle f(E) \rangle (\beta) = \sum_E f(E) P_\beta(E) / \sum_E P_\beta(E) \tag{1}$$

where we have used $\beta = 1/(k_B T)$. The probability histogram $P_\beta(E)$ of configurations with different energies can be obtained from the histogram at the reference temperature, $P_{\beta_0}(E)$

$$P_\beta(E) \sim P_{\beta_0}(E) \exp(-(\beta - \beta_0)E) \tag{2}$$

up to a normalization constant which cancels when $P_\beta(E)$ is used in Equation 1. The use of Equation 1 for reweighting has the disadvantage that one first needs to construct the histogram $P_{\beta_0}(E)$ and its properties are sensitive to how one discretizes the bins for values of E. Alternatively, one can use reweighting based on a time series of N measurements. It is even more general, as it can be used for any observable $\mathcal{O}$ which is a function of the configuration $\{s_i\}$ in the same time series. Equation 1 then translates to

$$\langle \mathcal{O} \rangle (\beta) = \left(\sum_{i=1}^N \mathcal{O}(\{s_i\}) \exp(-(\beta - \beta_0)E_i) \right) / \left(\sum_{i=1}^N \exp(-(\beta - \beta_0)E_i) \right) \tag{3}$$

In practice, reweighting provides reliable estimates close to the reference temperature but may completely fail further from it due to statistical errors.

Homework 2 (3 points)

1. Perform simulations using the (old) `ising` code at $T = 1.9$, 2.35 and 2.6 using the lattice size $L = 16$ and 5×10^5 sweeps.

2. Use the `reweight` program to apply the reweighting procedure to all three of your simulations. Use at least 30 target temperatures between $T = 1.7$ and $T = 2.8$.

3. Use the output of the `reweight` program to plot temperature dependence of susceptibility, $\chi = \beta N(\langle m^2 \rangle - \langle m \rangle^2)$, using the three different reference temperatures.

4. Why do the temperature dependences of susceptibilities differ when you use different reference temperatures?

5. Which of your reference temperatures should give the best estimate of the position of the peak in the plot?

6. Use the `histogram` program to obtain the histograms of energies from the simulations. Plot all histograms in one plot. Make one plot with linear and one with logarithmic scale on the y-axis to see better the parts with very low probabilities. *Hint: use n_bins=129, min=-2.00781, max=0.00781*

7. Based on the histogram, in which range of temperatures could you obtain reliable reweighting results with $T = 1.9$ as a reference temperature?

3 Parallel tempering

If the configurational space contains several minima separated by relatively high barriers, it may be difficult to sample the whole configurational space using standard (Metropolis) sampling techniques. A good example is the Ising model at low temperatures where the average absolute value of magnetization is $\langle |m| \rangle \approx 1$. By virtue of symmetry, both values of $m \approx 1$ and $m \approx -1$ are equally probable. But if the system is in one of these states, to get to the other one it would have to pass through states with $m \approx 0$ which have extremely low probability at low temperatures. In principle, we should obtain the correct value of $\langle |m| \rangle$ from a standard MC simulation if we could run long enough so that in the course of the run, we observe many flips from $m \approx 1$ to $m \approx -1$ and back. In practical terms, such a run would last for about a human lifetime and hence we would like to do something smarter. It would be a good idea to heat the system up to bring it to the region of $m \approx 0$ and then cool it down again. This approach is called simulated annealing. In this tutorial we will use another approach which is very similar in spirit and is called parallel tempering. We will run several simulations at different temperatures at once. After a certain number of sweeps, we attempt to swap configurations at neighbouring temperatures. The advantage of parallel tempering over simulated annealing is that it is trivially parallelizable and can take the advantage of multicore CPU architectures. Between the swapping attempts, simulations at different temperatures run independently and can be distributed to different CPUs, cores or threads.

Homework 3 (2 points)

The script `run_pt.sh` has redirected the output of `ising_pt` to `ising_pt.log` Apart from other output, you can find there the average values of various quantities for different temperatures. Time serries of magnetizations and energies for different temperatures are written to files `magnetization_pt.dat` and `energy_pt.dat`

1. Look at the script `run_pt.sh` and report the parameters of the parallel tempering simulation (temperatures, lattice size, number of steps, etc.).

2. Examine the function `swap_replicas()` in `ising_pt.c`. What criterion does it use to accept or reject the swap of configurations? Do not copy the code, describe it using a formula or in words.

3. In `ising_pt.log` you can also find the acceptance ratio of swapping the configurations at two neighbouring temperatures. What would you expect to happen if the neighbouring temperatures in the parallel tempering were further away from each other?

4 Comparison of the methods

Homework 4 (2 points)

1. Plot the time dependence of magnetization at temperature $T = 1.9$ in the range of sweeps 0 to 10^4. Make one plot for the standard MC and one for parallel tempering.

2. Use the `histogram` program to obtain the histograms of magnetization at temperatures $T = 1.9$, $T = 2.35$ and $T = 2.6$. Make one plot for the standard MC and one for parallel tempering.
   Hint: use n_bins=257, min=-1.0039, max=1.0039

3. Why do the time-evolution plots and histograms from different methods differ at some temperatures while they are similar at others?

Optional homework 1 (1 point)

These are things which look wierd at a first glance, but can be understood easily.

1. Why do we use 129 bins for the energy and 257 bins for the magnetization histograms? What happens if you use e. g. 100 or 400 bins?

2. Taking a closer look at the energy histograms at low temperatures, you may notice that approaching the value of -2.0 the histograms drops steeply to zero and then rises again to a finite value at $e = -2.0$. Still the probability value at $e = -2.0$ is about 10^2 times lower than the finite values next to it. Can you explain why it is so?

Optional homework 2 (2 points)

1. Modify the `reweight` program to use blocking or jackknife method and provide error estimates to the quantities obtained from reweighting.

2. Combine the temperature-dependences of susceptibility based on several reference temperatures using the error-weighted averaging (formula (13) and (14) in Ref. [2]).

References

[1] Histograms and All That, in: Computer Simulations of Surfaces and Interfaces, NATO Science Series, II. Vol. 114 (Kluwer, Dordrecht, 2003), pp. 137 - 157 `http://www.physik.uni-leipzig.de/~janke/Paper/histograms.ps`

[2] C. Holm and W. Janke, Phys. Rev. **B48** (1993) 936. If you are working on a CIP pool computer, you should be able to download the article from `http://prb.aps.org/abstract/PRB/v48/i21/p15807_1` or ask the tutor to provide a copy.